Simulating EUV Generation in Laser-Produced Plasma

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Howard Scott *Lawrence Livermore National Laboratory*
Frank McQuillan *University College Dublin*

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Co-conspirators

LLNL: Steve Langer, Dave Eder, Fred Hartemann, Jave Kane, Scott Wilks

LBNL: Alice Koniges, Kevin Gott

UCD: Padraig Dunne, Leanne Durkan, Oisin Maguire

Cymer: Mike Purvis, Igor Fomenkov, Alex Shafgans, Josh Brown, Daniel Brown

(Much of) This work performed under contract with Cymer

Outline

Part I

- Simulation requirements
- Simulation codes
- Atomic model
- Computational issues

Part II

- UCD Experiments

- Summary

The goal is to develop insight into the physics of laser-driven EUV generation, with the aim of developing a predictive computational capability

Physics requirements / Simulation issues

- Laser absorption
  - 1 µm (Nd:YAG) or 10 µm (CO_2)
- Energy transport via radiation, electron conduction, advection
- Hydrodynamics
- NLTE atomic kinetics
- EUV + other radiation production
- Radiation transport

- Resolution
  - Spatial mesh
  - Frequency mesh
  - Timesteps
  - Atomic structure
- Atomic model
  - Complexity
  - Accuracy
  - Expense

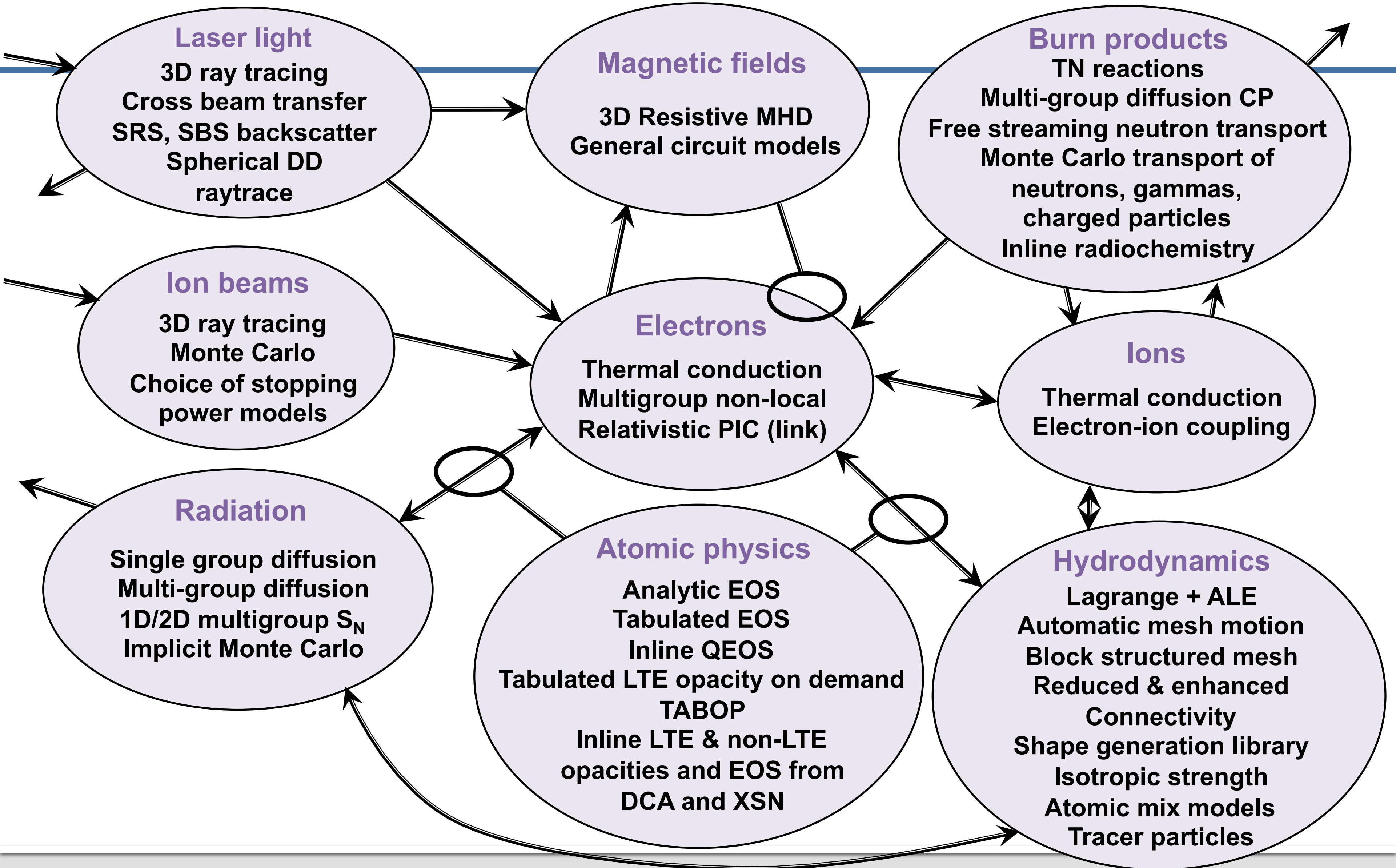
All physical processes must be consistent

Simulation codes

- Cretin
  - NLTE atomic kinetics
  - 1D / 2D / 3D radiation + line transport
  - 1D Lagrangian hydrodynamics
  - 1D laser ray trace and deposition
- HYDRA
  - 2D / 3D ALE (Arbitrary Lagrange Eulerian) hydrodynamics code
  - Implicit Monte Carlo radiation transport
  - 3D laser ray trace and deposition
  - Inline NLTE atomic kinetics (from Cretin)
  - Tabular or inline LTE / NLTE equation of state (EOS)
  - Massively parallel (>10^4 processors)

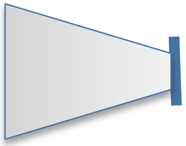
Well-established codes at LLNL now applied to EUV generation

Physical processes modeled by the HYDRA code



Simulation methodology

- 1D simulations
  - Run quickly in Lagrangian mode
  - Used for testing purposes and scoping studies
  - Expanding geometry (optional) mimics radial expansion



- 2D simulations
  - Capture radial expansion and laser profile
  - Require variable zoning, ALE strategy
  - Moderately-to-very expensive, depending on zoning detail + ALE
  - Emphasis on resolving important features
- 3D simulations
  - Extremely expensive
  - Reserved for non-axisymmetric investigations

A full study includes pre-pulse, drift, and main pulse phases (Purvis, et al, SPIE 9776, 2016)

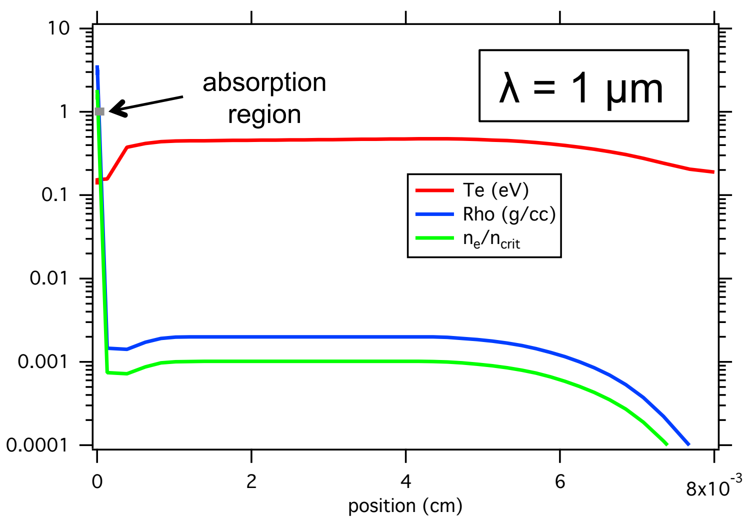
Laser wavelength: λ = 1 μm *vs* λ = 10 μm

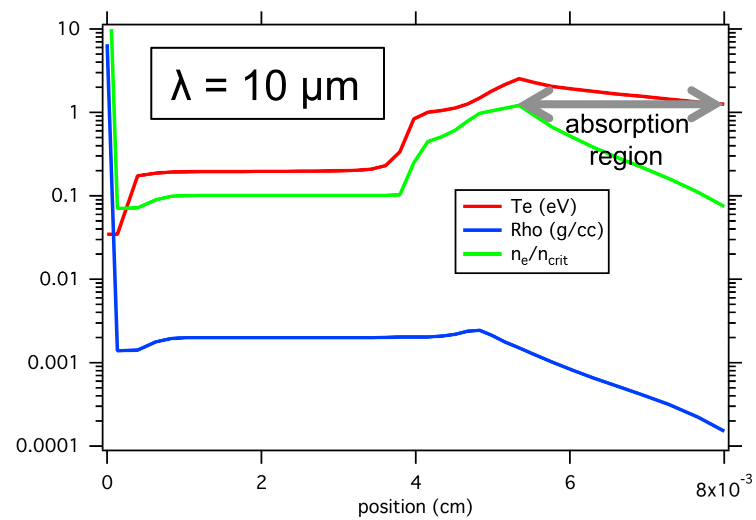
λ = 1 μm → $n_e^{crit} \approx 10^{21}$ cm^{-3}

- Absorbed energy conducts to higher density before being emitted as radiation
- Radiation emitted from very thin layer on steep temperature gradient
- Higher densities & optical depths

λ = 10 μm → $n_e^{crit} \approx 10^{19}$ cm^{-3}

- Energy is radiated very close to position of absorption
- Radiation emitted along absorption path length ~n_e^2 up to critical surface
- Lower densities favorable for 13.5 nm emission





LLNL laser-driven fusion uses λ = 1/3 μm

Atomic model construction

Configuration-averaged data calculated with FAC

- charge states with 28-50 electrons
- configurations 4s, 4p, 4d + $4f^1$,$4f^2$ + single excitations n=5-8 + double excitations to $5s^2$
  ~13000 levels, 2.5×10^5 radiative transitions
- UTAs for averaged radiative transitions

Detailed atomic structure / oscillator strengths calculated with FAC

- charge states with 28-50 electrons
  ~64000 levels, 2×10^6 transitions
- configurations 4s, 4p, 4d + $4f^1$ + single excitations n=5
- used to correct average data for configuration interaction effects

Wavelengths of 4d-4f, 4d-5f transitions corrected to match experimental data

Compact (screened-hydrogenic) atomic data calculated with Cretin

- charge states with 0-28 electrons - 330 levels
- matched to FAC data at Ni-like sequence

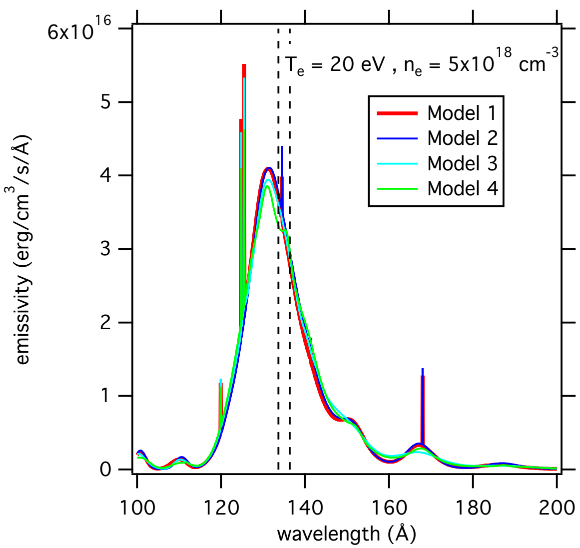
Incorporating NLTE atomic kinetics into rad-hydro

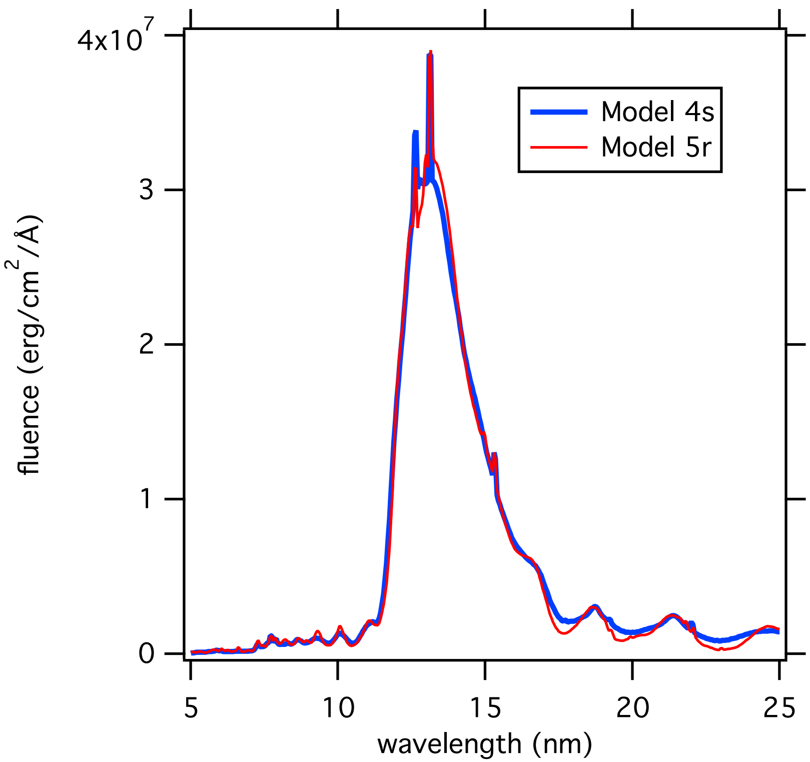
- HYDRA does NLTE atomic kinetics inline
  - uses radiative properties and EOS information
- Using the full atomic model is not possible
  - too expensive in CPU time and memory
- Our approach is to average / consolidate atomic data to produce an atomic model which can be run inline
  - ionization balance and emission spectra checked after each operation
  - EUV spectral fluence checked with 1D simulations
  - final atomic model ~10x faster but still uses ~80% of cpu time
- The goal is to minimize untested or uncontrolled approximations.

Inline atomic kinetics allows full coupling to other physics

Atomic model for rad-hydro simulations

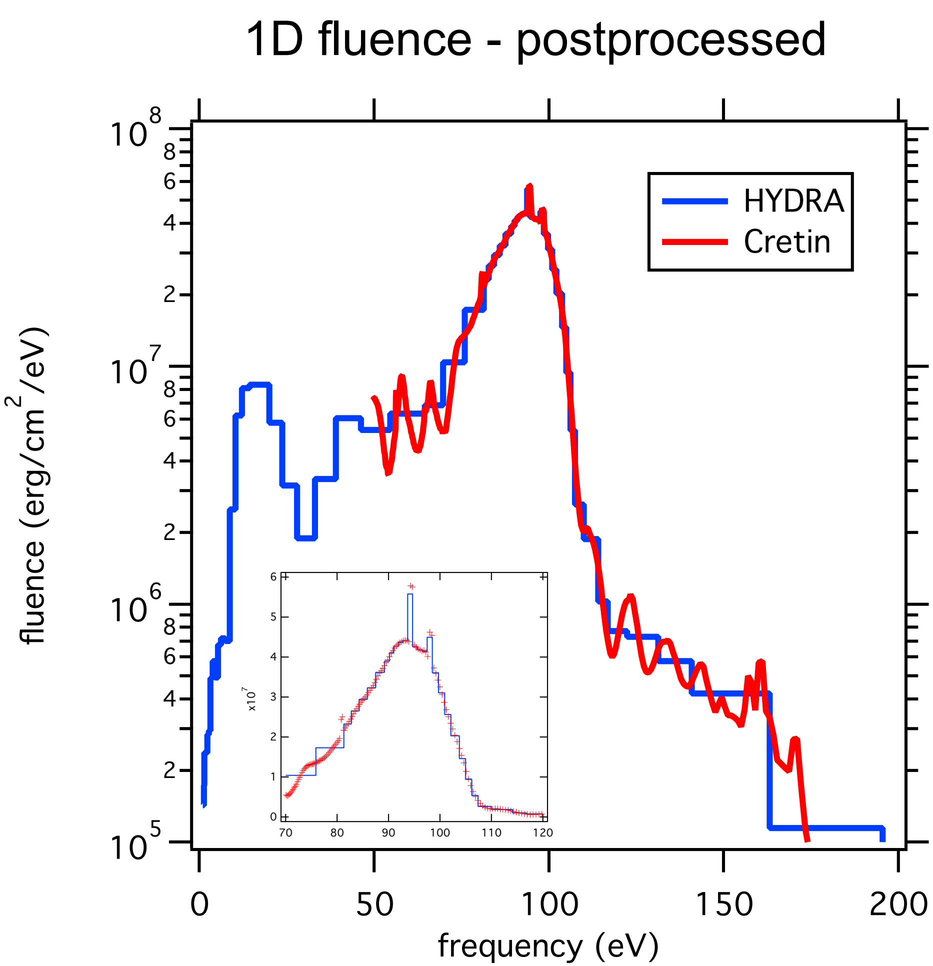
1) Start with full data
2) Average over principal quantum #'s for n>6
3) Average n=6 levels within ΔE= 1 eV
4) Combine n=5 levels within ΔE= 5 eV while retaining individual transitions





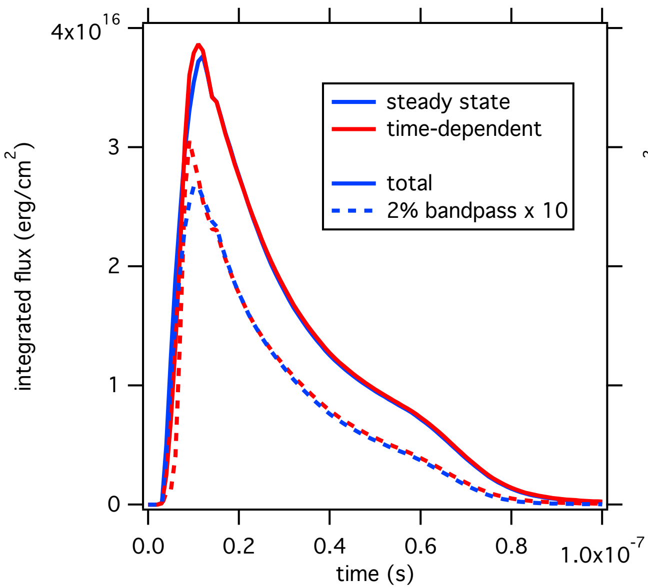
Frequency resolution

- HYDRA uses a frequency mesh designed to resolve the 13.5 nm bandpass and cover all radiative absorption and emission
  - 66 groups from 1 eV to 1 keV
  - Finely-spaced around 13.5 nm
- Cretin uses two frequency meshes:
  - HYDRA mesh for continuum
  - 480 groups from 10 nm to 250 nm for spectral output
- HYDRA has sufficient resolution for energetics + transport of bandpass radiation, but not for the full spectrum

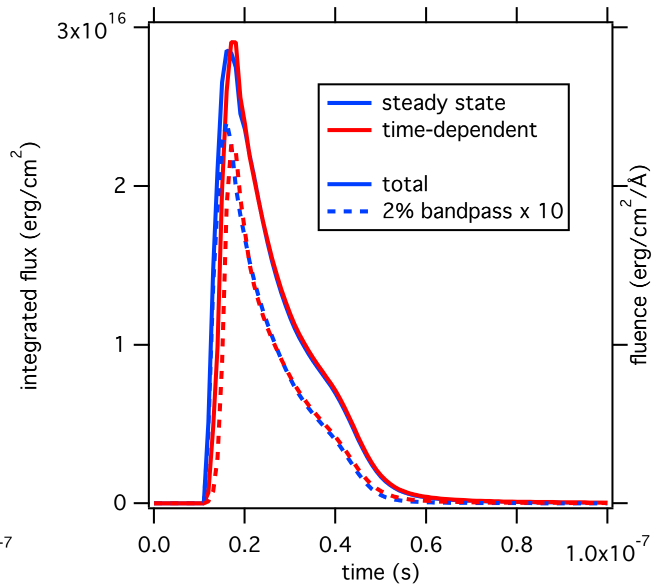


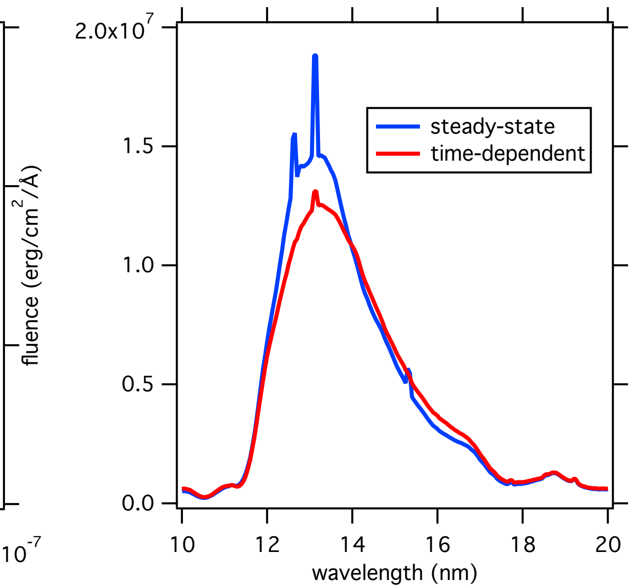
Time-dependent or steady-state kinetics?

- Inline kinetics are run in a time-dependent mode
- Postprocessing can use either time-dependent or steady-state mode
- Validity of steady-state kinetics is necessary for a tabular approach



100 ns pulse





50 ns pulse, 2x intensity

A fast-rising pulse requires a time-dependent treatment

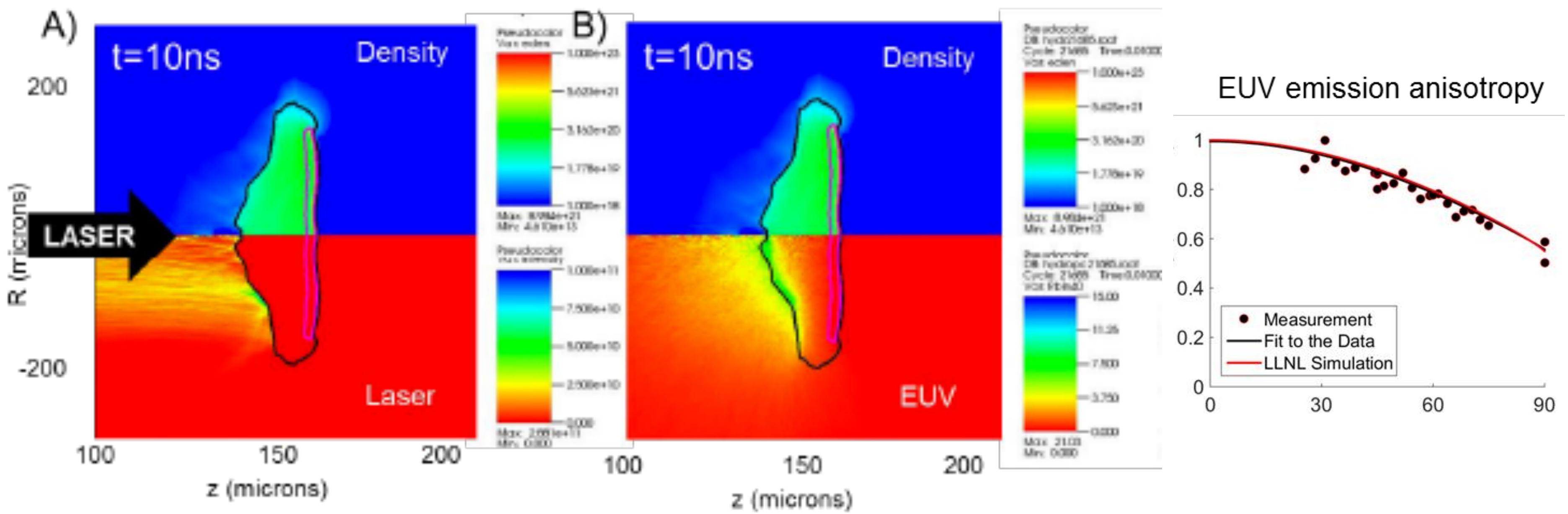
Further investigations

- 1D simulations varying laser pulses
- 2D simulations varying pulse profiles
- 3D simulations varying angle of incidence

- Tabular approach
  - Applied after pulse rise when steady-state kinetics is valid
  - Low density in emitting region → low optical depth for escaping radiation
  - Optically-thin information should be accurate (not true for $\lambda = 1\ \mu m$!)
  - Tabular approach testing showed good agreement with 1D simulations
  - Possible speed-up of ~5x

2D main pulse simulation

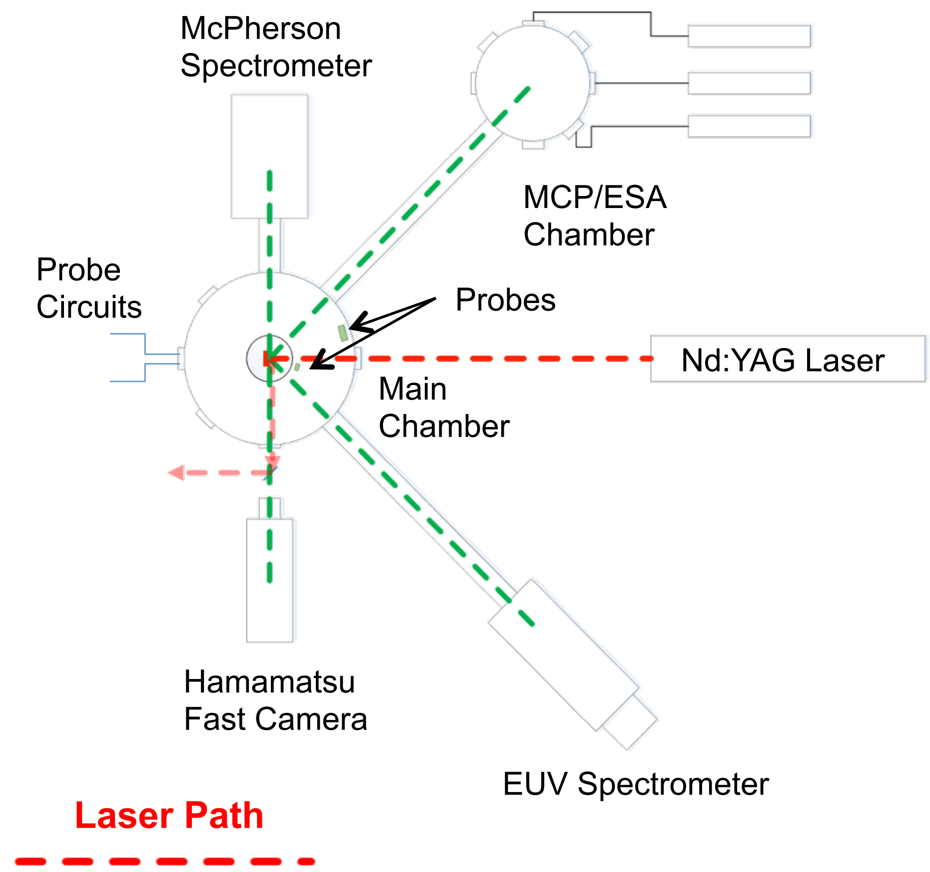
- Early time (or pre-pulse) ablation produces large region of low-density plasma
- Laser energy is absorbed up to critical surface, away from target surface
- EUV emission comes from region of laser absorption, primarily from 0.1-1 n_{crit}



Purvis, et al, SPIE 9776, 2016

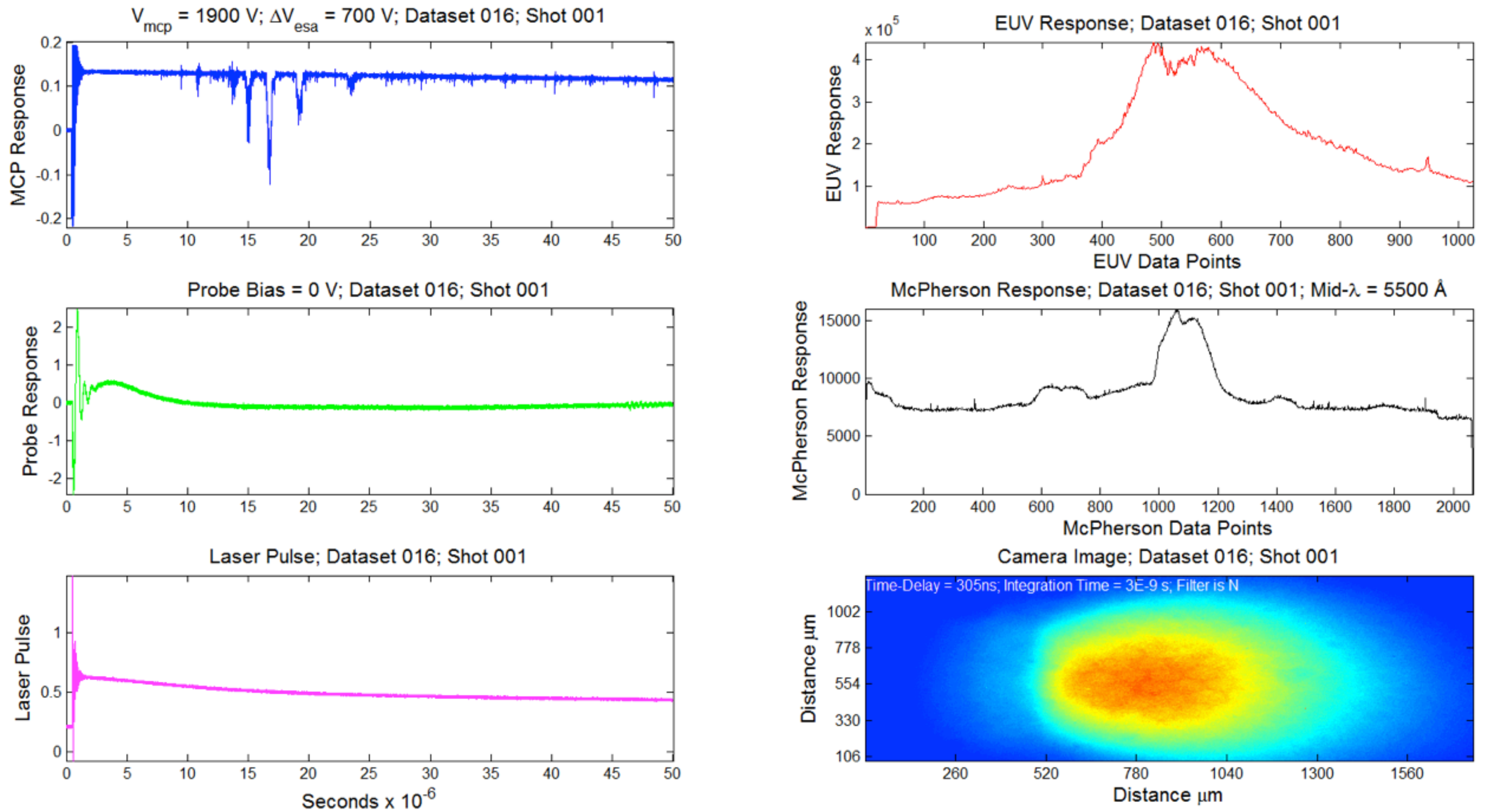
UCD planar target experiments

- Dual probes at variable distances from target measure arrival of charged plasma
- Time-of-flight identifies charge states
- Analysis produces charge state distribution vs. distance
- Spectral analysis complements charge state analysis



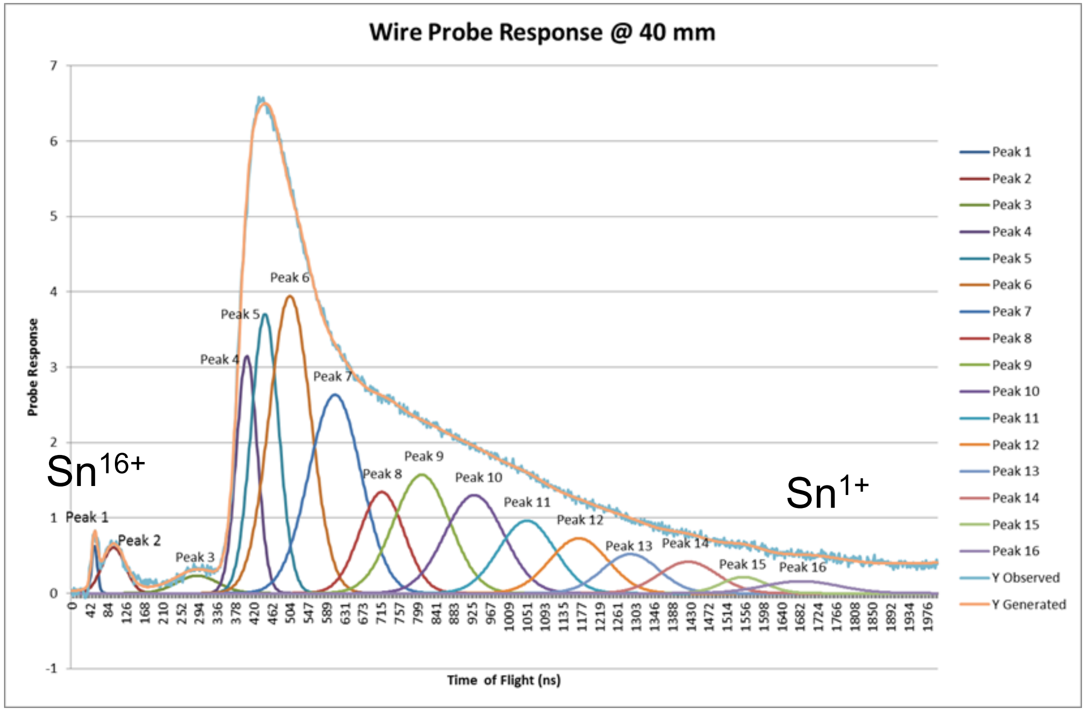
Simultaneous multi-sensor characterization of Sn laser plasma

Data set includes multiple diagnostics



Time-of-flight analysis identifies charge states

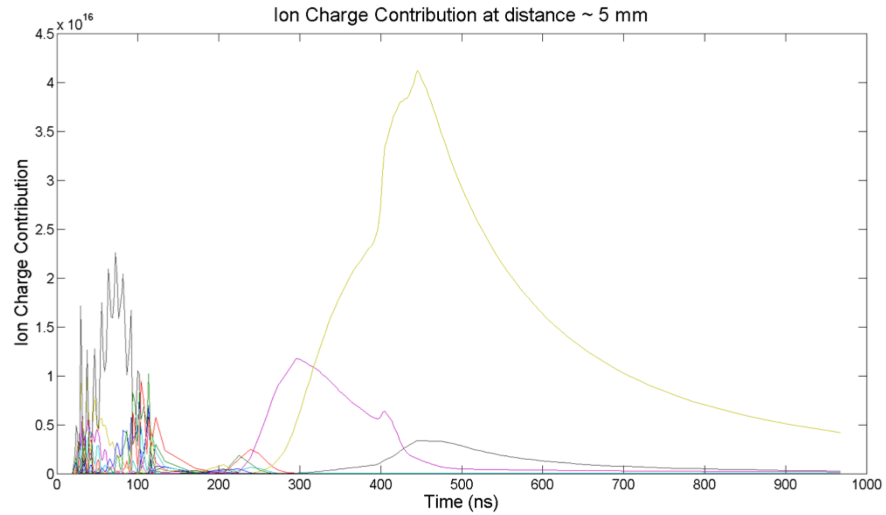
- Varying probe distance from target scans charge state fractions vs. time
- Deconvolution produces charge state distribution vs. position for comparison with simulations

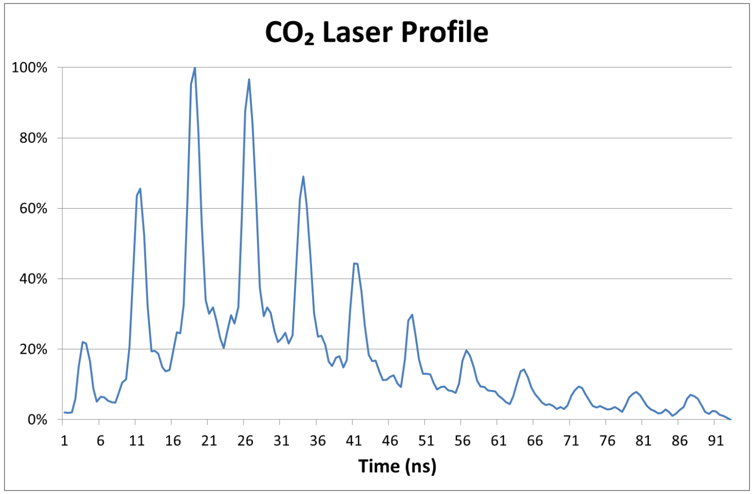


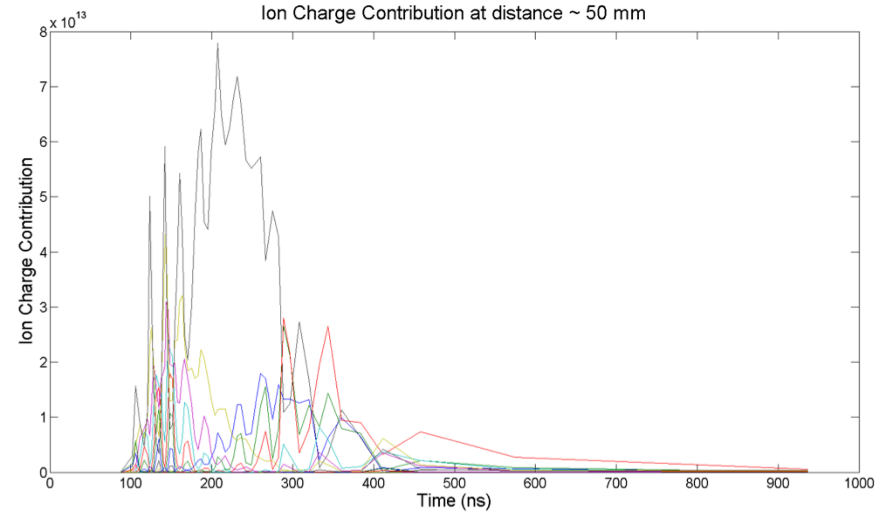
Simulations predict evolving charge state distributions in space and time

<u>1D rad-hydro Cretin simulations</u>

- Laser pulse shape imprints on charge state distributions
- Rapid initial evolution for highly-charge states
- Slower evolution at larger distances for more neutral states

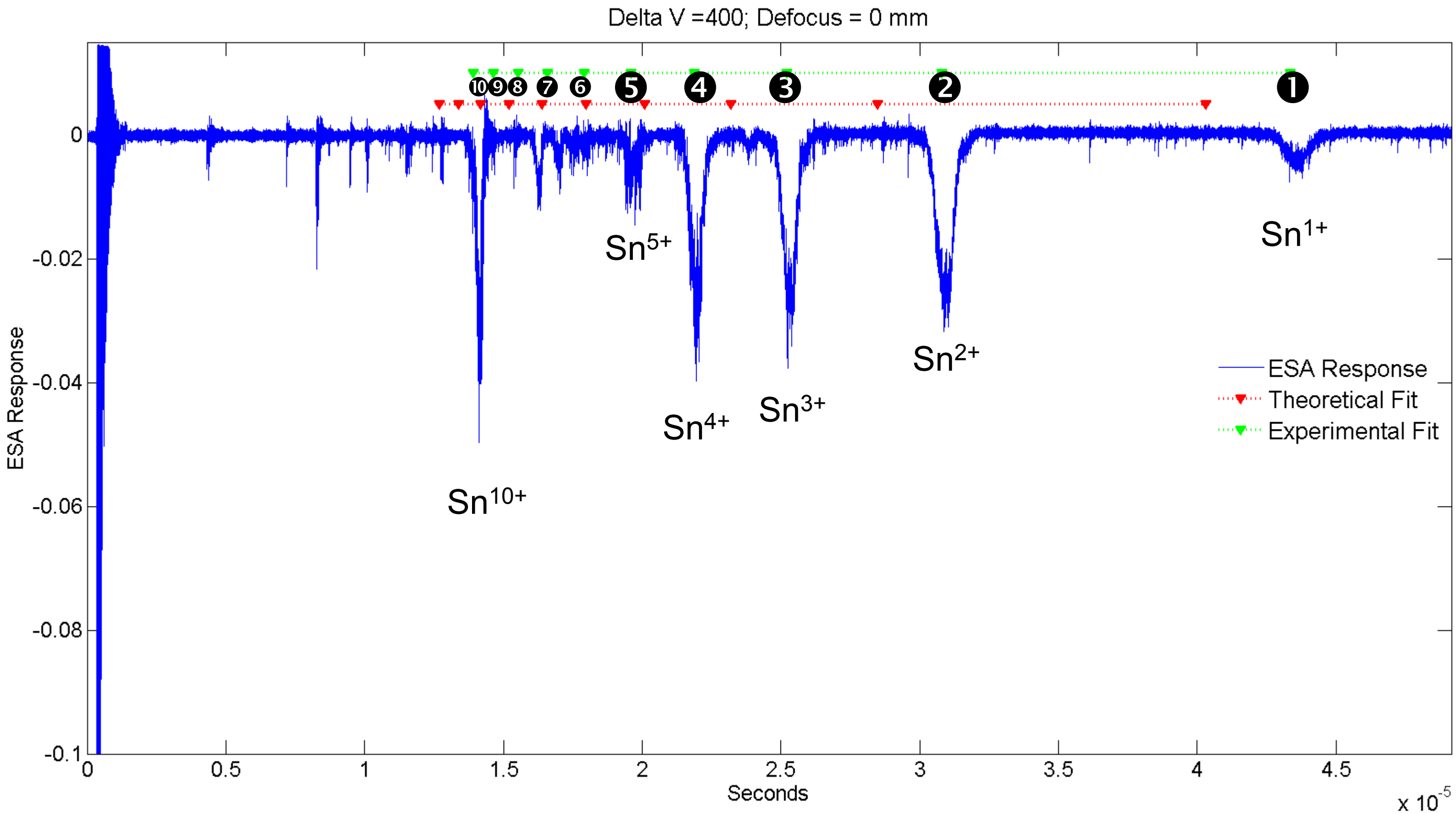






MCP / Energy Sector Analyzer experiments

- Voltage + time of flight identifies charge states
- Signal strength produces relative population



Summary

LLNL codes are being applied to EUV production

- Including microphysics of EUV generation
  - laser absorption, NLTE kinetics, hydrodynamics, radiation transport, conduction
- Aiming to resolve important length / time / frequency scales
- Aiming to minimize uncontrolled approximations
- Applying to laboratory experiments
- Addressing experimental diagnostics

We are gaining experience with EUV simulations and progressing towards a predictive capability

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Abstract

Radiation-hydrodynamics simulations of radiative emission from laser-produced plasmas require modeling multiple macroscopic physical processes with an accurate treatment of the underlying atomic physics. Basic temperature, density and spatial scales follow from the laser parameters and material properties, determining the general computational approach, but capturing important features with high fidelity and matching experimental diagnostics often calls for specialized techniques.

We discuss experiences with and developments from simulations of EUV generation done at LLNL and UCD over the last few years. Common goals of these efforts included identifying critical physical processes and developing a predictive modeling capability. The modeling at UCD used Cretin [1] for 1D simulations of Sn plasmas driven by Nd:YAG and CO_2 lasers. The LLNL modeling, done in collaboration with Cymer, used HYDRA [2] for a series of 1D, 2D and 3D simulations of Sn droplets driven by a CO_2 laser prepulse and main pulse.

[1] H. A. Scott, J. Quan. Spectrosc. Radiat. Transf. **71**, 681 (2001).

[2] M.M. Marinak, G.D. Kerbel, N.A. Gentile, O. Jones, D. Munro, S. Pollaine, T.R. Dittrich, S.W. Haan, Phys. Plasmas **8**, 2275 (2001).